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13. ABSTRACT (Maximum 200 words) During the period April 89-90, we carried out experiments on studies of hetero-epitaxial films grown on lattice-mismatched substrates in three main areas: (1) migration-enhanced (or modulated) MBE to promote 2-dimensional growth of hetero-epitaxial films, (2) growth on patterned substrates to reduce thermal stress, and (3) study of GaAs/Si laser characteristics, especially polarization dependence and threshold current, to correlate with results from basic material studies in area 1 and 2. Recently we have started exploring new directions for hetero-epitaxy on lattice-mismatched substrates, and have done exploratory work on (4) growth on (111) plane of strained AlInAs/AlAs quantum well and (5) GaAs growth on Si/sapphire (SOI) substrate. In this report, we first summarize experimental results on work in groups 1, 2 and 3. This is followed by a discussion of our exploratory work which will point the direction for our future research. J316				
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# TECHNICAL PROGRESS REPORT

April 89-90

(AFOSR-88-0174)

Studies of Hetero-Epitaxy of GaAs Films on Si Substrate  
for Effective Control of Defect Density and Internal Stress

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During the period April 89-90, we carried out experiments on studies of hetero-epitaxial films grown on lattice-mismatched substrates in three main areas: (1) migration-enhanced (or modulated) MBE to promote 2-dimensional growth of hetero-epitaxial films, (2) growth on patterned substrates to reduce thermal stress, and (3) study of GaAs/Si laser characteristics, especially polarization dependence and threshold current, to correlate with results from basic material studies in area 1 and 2. Recently we have started exploring new directions for hetero-epitaxy on lattice-mismatched substrates, and have done exploratory work on (4) growth on (111) plane of strained AlInAs/AlAs quantum well and (5) GaAs growth on Si/sapphire (SOI) substrate. In this report, we first summarize experimental results on work in groups 1,2, and 3. This is followed by a discussion of our exploratory work which will point the direction for our future research.

### *1. Migration-Enhanced (or Modulated) MBE*

Refer to publications [1-3] for details. As reported in the last progress report, nominal 150 Å-thick GaAs films were grown on Si substrates by modulated MBE and conventional MBE for comparison. Structural characterizations by plan-view and high-resolution TEM show that the nucleation of GaAs film grown by modulated MBE is more 2-dimensional than that grown by conventional MBE [1-2]. Furthermore, using modulated MBE for the initial layer growth, it was found that the PL intensity of 3 μm-thick films is 80% higher than that of films grown by conventional two-step MBE. The x-ray diffraction FWHM is also narrower (250 versus 300 arcsecond) [1,2].

Since the last progress report was submitted, we have carried out an extensive analysis of the experimental results and performed additional high-resolution TEM to examine the interfacial defect structure [3]. It is found that the Moire fringes elongate along a fixed direction with reference to the Si substrate and that the direction of elongation is parallel to the step edges of the tilted Si substrate. These observations are in agreement with the generally accepted view that nucleation starts at these step edges. High-resolution TEM shows a high density of stacking faults and microtwins originating from the interface instead of type I or type II dislocations. Since the nature of interfacial defects is a central issue determining the film quality during subsequent growth, an analysis is undertaken, based on the strain energy relieved  $\Delta E_s$  and the energy of dislocation formation  $\Delta E_d$ .

The two energies depend on the Burgers vector  $\vec{B}$ , the dislocation line direction  $\vec{U}$ , and the crystal orientation. The results of our analysis for growth on (100) plane can be summarized as follows. During the initial growth prior to thermal annealing, type I dislocations have the largest ratio of  $\Delta E_s/\Delta E_d$ . On the other hand, type II can dissociate into two Shockley partials, one of which has the same ratio  $\Delta E_s/\Delta E_d$  as, but a much smaller formation energy  $\Delta E_d$  than, the type I dislocation. Therefore, from the energetic point of view, the partials are more likely to be generated than type I dislocations during the initial growth. When the two partials glide on the  $(\bar{1}\bar{1}1)$  plane, they leave a stacking fault in between. This is what we detect from high-resolution TEM.

The main difference between modulated and conventional MBE is that more complicated defect structure than the V-shaped stacking fault is formed and observed during the initial growth by conventional MBE. It is apparent that the smaller island size

of the modulated MBE is more favorable to the formation of simple V-shaped stacking fault at the places when two islands coalesce. Upon subsequent thermal annealing, most V-shaped stacking faults and partials are converted back into type II dislocations, but defects of more complicated structures are more difficult to be annealed out.

The results of our study of the modulated MBE can be summarized as follows. With a more 2-dimensional growth mode, the nucleation density is increased and the spacing between the nucleated islands is reduced. This leads to the formation of many V-stacking fault pairs which can be annealed out to form a single type I dislocation. Equally important, a continuum coverage of the epitaxial film during the early stage of growth forces the interaction and cancellation of partial dislocations to occur at a distance closer to the interface than that in the case of a 3-dimensional island growth. This means that the thermal energy required to anneal out these partial dislocations is lower in a 2-d growth than in a 3-d growth. Both factors lead to improved quality of the film grown by modulated MBE.

## 2. *Growth on Patterned Substrate and SLS Buffer*

Refer to publications [4,5] for details. In the last progress, we reported low-temperature PL studies of GaAs films grown on SiN-patterned Si substrates (*Appl. Phys. Lett.*, Vol. 52, p. 215, 1988) and GaAs films etched into mesa stripes with free standing walls (*Appl. Phys. Lett.*, Vol. 53, p. 2394, 1988). In the former, films grown on patterned substrates show enhanced PL intensity as compared to films grown on planar substrates. In the latter, films with standing walls show significant relief of thermal stress. Continuing our effort of exploring possible ways to reduced threading dislocation density and to relieve thermal stress in the GaAs films, we have introduced

strained-layer superlattices (SLS) as buffer [4,5] and grown raised-mesa of GaAs film on SiN-patterned Si substrates [5]. The results are very encouraging.

For the GaAs/InP films, the buffer layer structures under study are (a) GaAs layer grown at low temperature, (b) low temperature GaAs layer plus two sets of 5-period  $\text{In}_{0.08}\text{Ga}_{0.92}\text{As}/\text{GaAs}$  SLS and (c) a compositionally graded  $\text{In}_x\text{Ga}_{1-x}\text{As}$  layer with  $x$  varying from 0.53 (for lattice-match to InP substrate) to  $x=0$  plus 2 sets of 5-period InGaAs/GaAs SLS. Figures 1 and 2, taken from publication 4, show the buffer structure and the measured 77K PL intensity of the various films. The film with SLS buffer shows the highest PL intensity and narrowest PL linewidth. Furthermore, cross-sectional TEM study reveals significant bending of threading dislocations by SLS, especially at the second set of SLS placed at  $1\mu\text{m}$  from the hetero-interface. Therefore, the improved optical quality of the thick GaAs film can be attributed to a significant reduction of threading dislocation density in the film through bending.

As a continuation of our effort in stress relief and dislocation-density reduction, we have grown GaAs films on SiN-patterned (100) Si substrates without and with  $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}$  SLS (3 periods). The GaAs films grown from SiN openings in the form of raised mesas have free standing side walls, relieving thermal stress. Figures 2-5, taken from the preprint of publication [5], show, respectively, 77K PL spectra, residual stress as deduced from the PL peaks, etch pits, and etch-pit density of the films grown on mesas of different size. A significant reduction in both residual stress and etch-pit density is observed for mesa size  $L < 45\mu\text{m}$ . The residual stress is reduced to below  $1 \times 10^9 \text{ dynes/cm}^2$  for the  $L=8\mu\text{m}$  mesa. The etch-pit density is reduced to  $7 \times 10^6 \text{ cm}^{-2}$  in the  $L < 45\mu\text{m}$  mesas without SLS and further reduced to  $1.2 \times 10^6 \text{ cm}^{-2}$  in the  $L=45\mu\text{m}$  mesa with SLS.

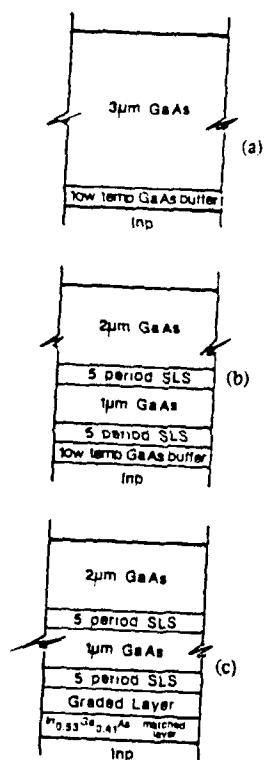


Fig. 1 Schematics of different buffer structures: (a) Low temperature grown GaAs buffer layer; (b) 2 sets of  $\text{In}_{0.05}\text{Ga}_{0.95}\text{As}/\text{GaAs}$  SLS; (c) Transitional graded  $\text{In}_x\text{Ga}_{1-x}\text{As}$  layer plus 2 sets of  $\text{In}_{0.05}\text{Ga}_{0.95}\text{As}/\text{GaAs}$  SLS.

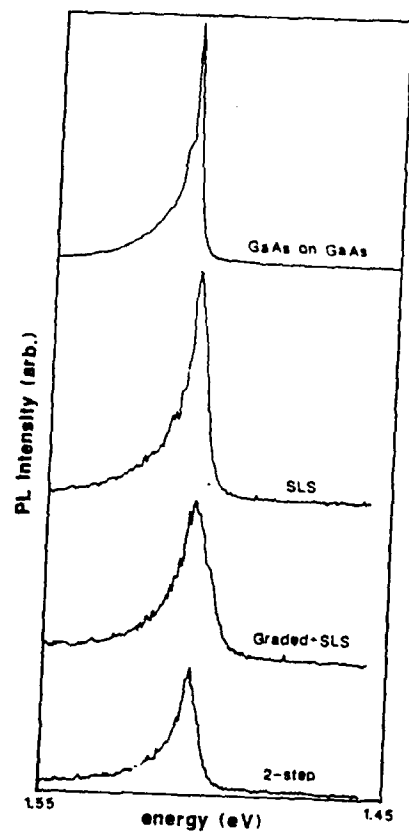


Fig. 2 77K photoluminescence spectra from GaAs on InP and GaAs on GaAs films. The spectrum from GaAs on GaAs film is in different scale.

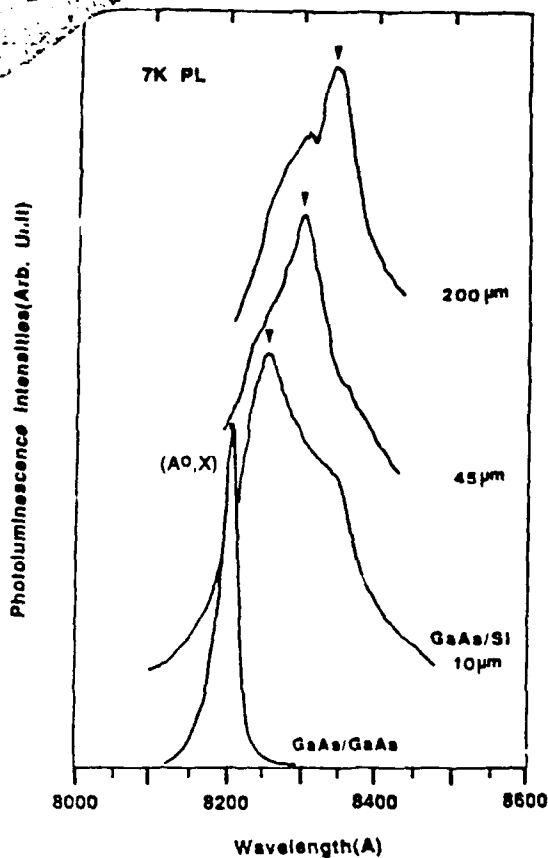


Fig.2 Photoluminescence spectra from as - grown GaAs films on patterned Si substrates with varying mesa size.

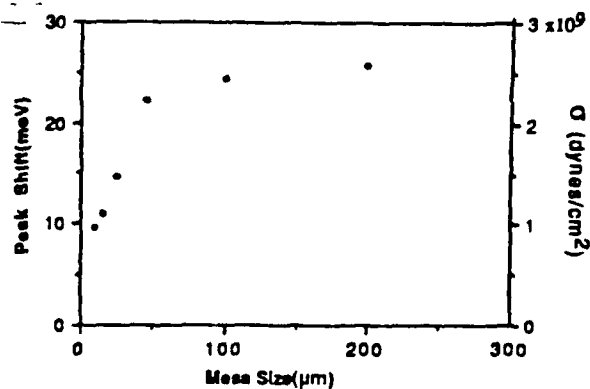


Fig.3 Shift of the photoluminescence peaks and the residual stress in GaAs layers as a function of the mesa size.

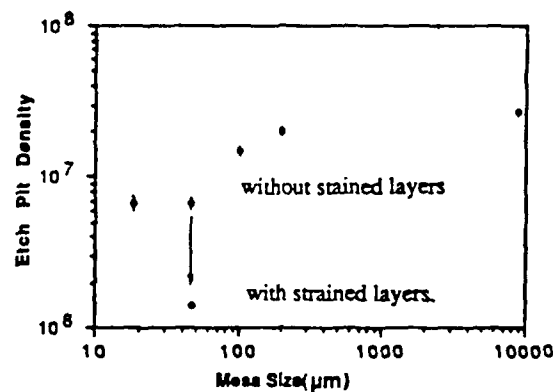


Fig.5 Etch pit densities as a function of mesa size

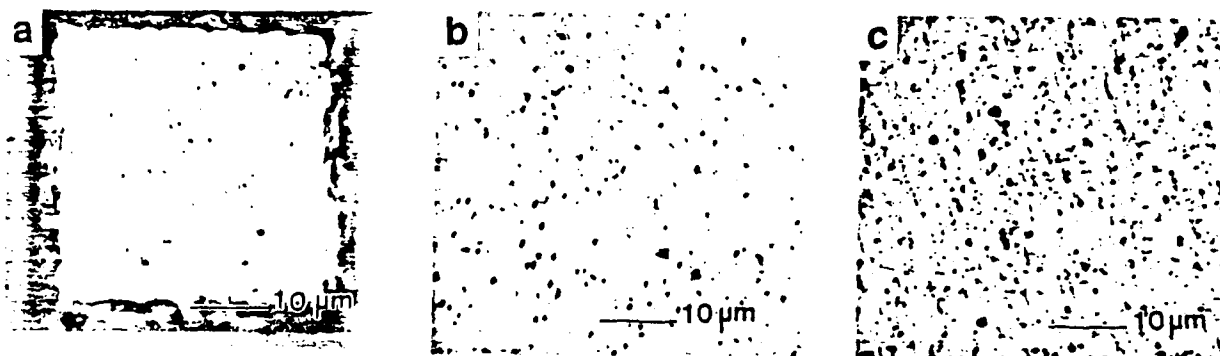


Fig.4 Optical photographs showing etch pits on GaAs epilayers grown on mesas of different size. (a)  $L = 45 \mu\text{m}$  (b)  $L = 100 \mu\text{m}$  (c) unpatterned

masks were designed so that the total mesa area was larger than that of the region between mesas. As the mesa size decreased, the position of the strong peak moved towards that of GaAs/GaAs. Figure 3 shows the shift of the main peak of GaAs/Si with respect to that of unstrained GaAs/GaAs as a function of mesa size. The peak shift decreased with decreasing the mesa size, which means the residual stress in GaAs on mesas was reduced considerably by reducing the mesa size. The biaxial tensile stress in GaAs on  $200 \mu\text{m}$  mesas was estimated to be  $2.7 \times 10^9 \text{ dynes/cm}^2$  using  $\Delta E / \sigma = 10.2 \text{ meV} / (1 \times 10^9 \text{ dynes/cm}^2)$  [5] for the light hole valence band shift. This high biaxial tensile stress was reduced to below  $1 \times 10^9 \text{ dynes/cm}^2$  when the mesa size was reduced to  $L = 8 \mu\text{m}$ .

The results are significant in determining the potential usefulness of hetero-epitaxy on lattice-mismatched substrates for future opto-electronic integration and laser applications. In this regard, the following observations are appropriate. Defect generation and propagation have been studied in InP light emitting diodes under a uniaxial stress [M. Iwamoto and A. Kasami, *Appl. Phys. Lett.*, Vol. 28, p. 591, 1976; M. Ogura et al., *Jpn. J. Appl. Phys.*, Vol. 20, p. L363, 1981]. It has been found that at a forward current of 20 mA, a uniaxial stress of  $1.5 \times 10^9$  dynes/cm<sup>2</sup> is required to generate dark line defects, and at a current of 50 mA, the required stress is reduced to  $8 \times 10^8$  dynes/cm<sup>2</sup>. With the use of quantum wells, a semiconductor laser can have threshold current well below 10 mA. Therefore, the reduction in residual stress to below  $10^9$  dynes/cm<sup>2</sup> may make the technology viable for growing laser-quality films on lattice-mismatched substrates. We also note that at a dislocation density of  $10^6$  cm<sup>-2</sup>, a laser of cross-sectional area  $(10 \mu\text{m})^2$  intersects on the average one dislocation line, which is of the same order of magnitude as the dimension of surface emitting lasers. In our laboratory, we have made surface emitting lasers with a lateral dimension less than  $10 \mu\text{m}$  and a threshold current of 15 mA even without using QW as the active layer. Therefore, the numbers regarding residual stress and dislocation density are promising for applying the technology to semiconductor lasers.

### 3. GaAs Lasers Grown on Trenched and Raised-Mesa Si Substrates

Refer to publications [6-10] for details. Ultimate test of the optical quality of films grown on lattice-mismatched substrates is the attainment of laser action. Information concerning the dislocation density and the residual stress can be inferred from the operating life and the polarization characteristic of such lasers. In the last progress

report, we described preliminary results on GaAs/GaAlAs lasers grown on SiN-patterned Si substrates [6]. Since then, we have made extensive measurements, and completed an analysis, of the polarization characteristics of such lasers [7]. Because of the long stripe geometry of the laser, the stress in the plane of the active layer is expected to be nonuniform, and hence can be decomposed into a uniaxial stress and a uniform biaxial stress. The latter component favors the polarization parallel to over the polarization perpendicular to the stress symmetry axis with a ratio of 4 to 1 for the matrix elements  $|M|^2$ . Since the symmetry axis for a uniform biaxial stress is normal to the active layer, the TM polarization is favored over the TE polarization. Only in stripe-geometry lasers where uniaxial stress dominates, the TE polarization prevails over TM polarization because mirror reflectivity is higher for TE mode than for TM mode. This happens in lasers with stripe width  $L < 10 \mu\text{m}$ .

The threshold current density for the GaAs laser on SiN-patterned substrate with an active-layer thickness of  $0.16 \mu\text{m}$  is  $4.5 \text{ kA/cm}^2$ , and the laser has a differential (slope) efficiency of 27% [7,8]. Both numbers show that the GaAs/Si laser performance, though somewhat inferior to that of GaAs/GaAs laser, is reasonably good. One serious problem with the GaAs/Si laser is the short operating life. Under pulse operation, the laser can last for a long time (that is, the laser is still working after repeated measurements. Under CW operation, however, the laser lasts only for few minutes. Because the active layer is surrounded by polycrystalline GaAs and GaAlAs and removed from the substrate by almost  $5 \mu\text{m}$  (the combined thickness of the buffer and cladding layers), heating is a serious problem, and we believe is a major contributor to performance degradation under CW operation. If we use  $150 \text{ \AA}$  quantum well for the active layer, we can expect a reduction of threshold current density  $J_{\text{th}}$  from

4.5 kA/cm<sup>2</sup> to below 500 A/cm<sup>2</sup>, resulting in a much lower threshold current and hence a much less heating problem. For  $J_{th}=500$  A/cm<sup>2</sup>, the threshold current is only 4 mA in a laser of typical 3  $\mu$ m  $\times$  250  $\mu$ m dimension. The value is well below the current of 20 mA to initiate generation of dark line defects at an internal stress of  $1.5 \times 10^9$  dynes/cm<sup>2</sup>.

Encouraged by the results, we have grown three types of GaAs/Si laser structures: (1) planar, (2) mesa, and (3) selective-area (or SiN-patterned), and studied their polarization characteristics [9,10]. Figures 1 and 2, taken from the manuscript to be submitted for publication, show the structure and polarization characteristic of these lasers. At the outset, we should point out the difference in heat treatment for the various lasers and its obvious effect on the polarization characteristics. There are two groups of planar lasers with group 2 having undergone sintering at 400°C for 10s after the wafer is lapped down to about 100  $\mu$ m in thickness. The group 2 (GaAs/Si) lasers have polarization characteristic almost identical to the GaAs/GaAs (group 5) lasers. The group 1, group 3 and group 4 GaAs/Si lasers were not subject to heat treatment. The selective-area (SiN-patterned, group 4) GaAs/Si lasers have identical structures as those reported in [7,8] except that the laser structures in [7,8] were annealed in MBE chamber while those of group 4 were not. The thermal annealing consisted of five cycles during which the substrate temperature was raised to 700°C for 5 minutes and then lowered to 450°C for another 5 minutes. While the in-situ annealed selective-area lasers with  $L < 10 \mu$ m show predominantly TE polarization as previously described, the unannealed selective-area lasers show persistent TM polarization. The group 3 (mesa) GaAs/Si lasers, however, like the group 1 GaAs/Si lasers, have stronger TE polarization than TM polarization even without heat treatment.

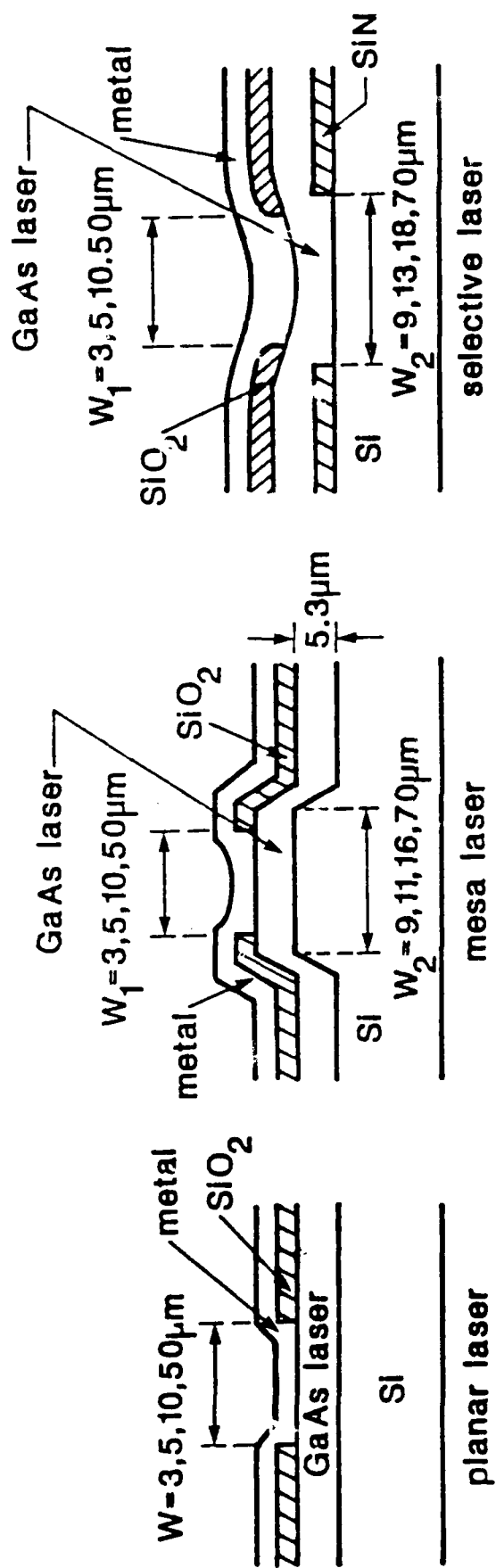
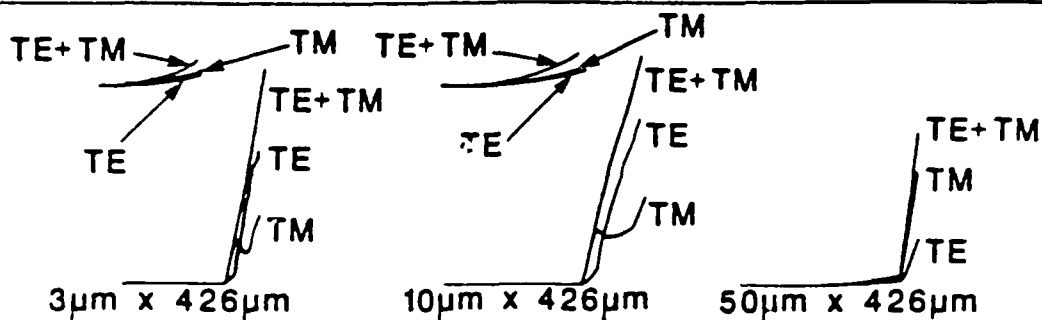


Fig 1

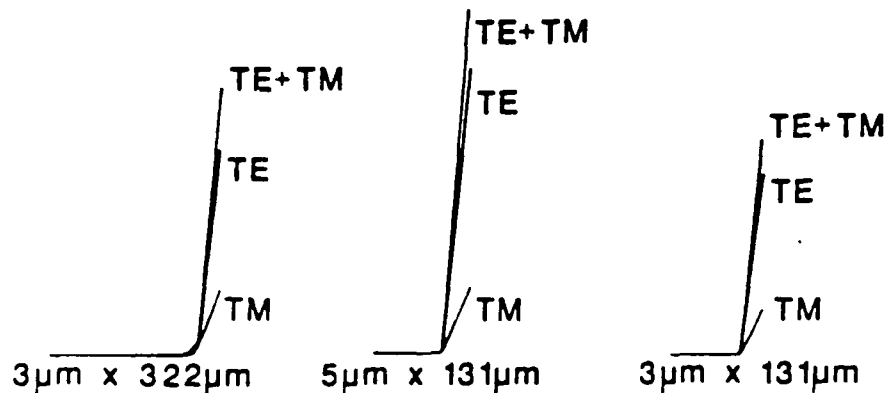
Group 1

planar before  
annealing



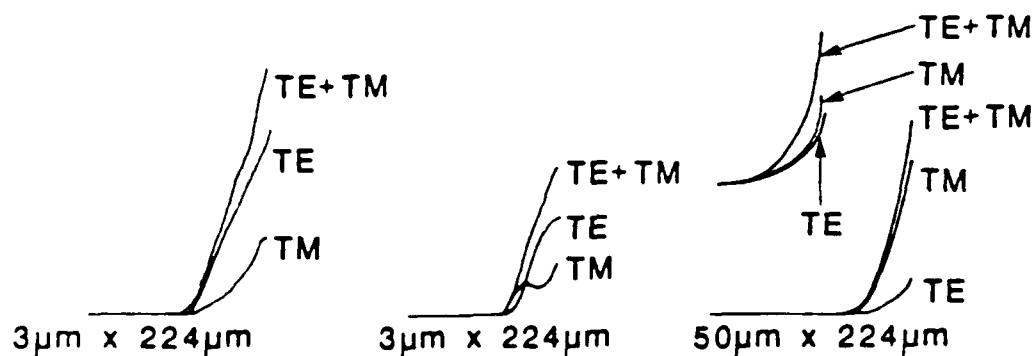
Group 2

planar after  
annealing



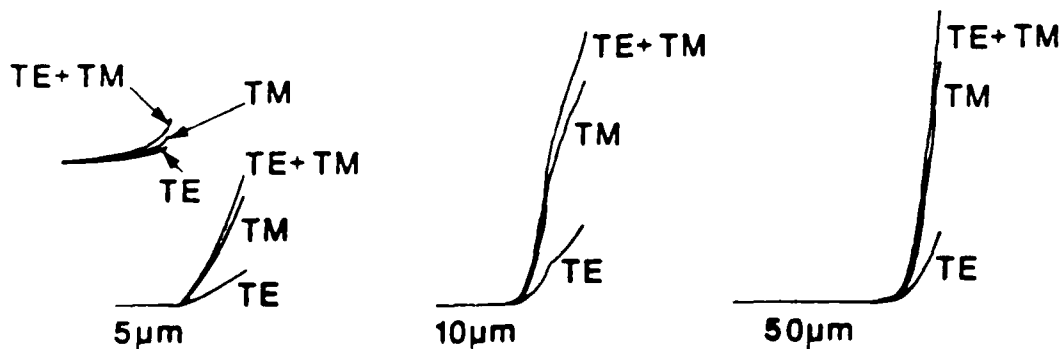
Group 3

Mesa



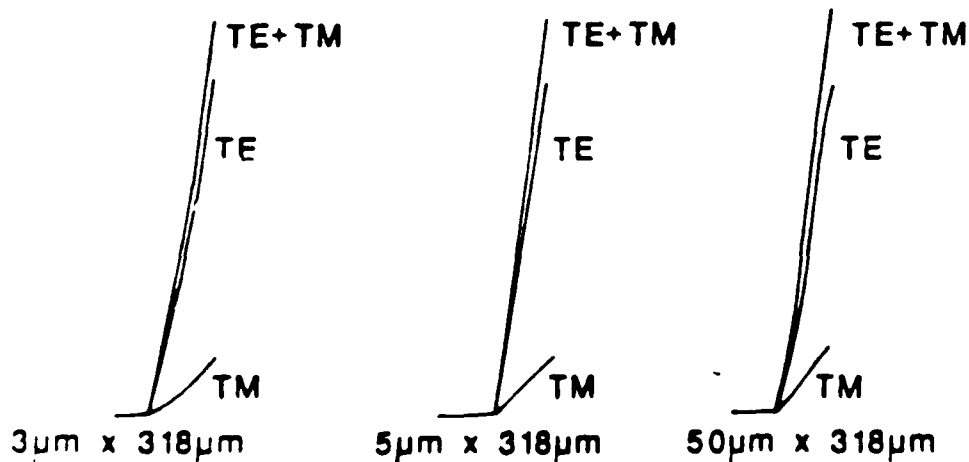
Group 4

Selective



Group 5

GaAs/GaAs



One problem with the selective-area (SiN-patterned) lasers is the necessity of using RIE to remove SiN for window opening. The step has somehow smeared the regularity of atomic steps in the misoriented Si substrate [6]. In contrast, there is no mask required in growing planar- and mesa-type GaAs/Si lasers. Furthermore, the thermal path for heat dissipation is not restricted in these two structures. In future investigations we'll concentrate on these two structures.

In summary, measurements of PL spectra and etch-pit densities have shown that the residual stress can be reduced to below  $10^9$  dynes/cm<sup>2</sup> and the dislocation density can be reduced to around  $10^6$  cm<sup>-2</sup>. Measurements of GaAs/Si laser performance have yielded equally encouraging results. They show a reasonably good slope efficiency (27%), exhibit a predominantly TE polarization, and indicate a threshold current below 10 mA if quantum well is used. These results are obtained without having the growth procedure and laser structure optimized. We believe that the combined use of QW, SLS, in-situ thermal cycling, and post-processing annealing at low temperature should further improve the GaAs/Si lasers performance and greatly slow down degradation rate of these lasers.

In preparation for future research, we have done exploratory work in two areas: (1) heteroepitaxy of AlInAs/AlAs and GaAs/GaInAs/Si films and (2) heteroepitaxy of GaAs/Si/SiO/Si and GaAs/Si/sapphire films. One important question regarding hetero-epitaxy is the quality or controlled purity of the substrate surface. It is known that the Si wafer for VLSI has to be denuded of oxygen near the surface where epitaxy takes place. The oxide removal procedure step generally followed in GaAs/Si growth is far less stringent than that used in VLSI procedure. Our aim is to have an oxygen-free Si surface layer of at least few hundred angstrom thick. The oxygen-free Si layer

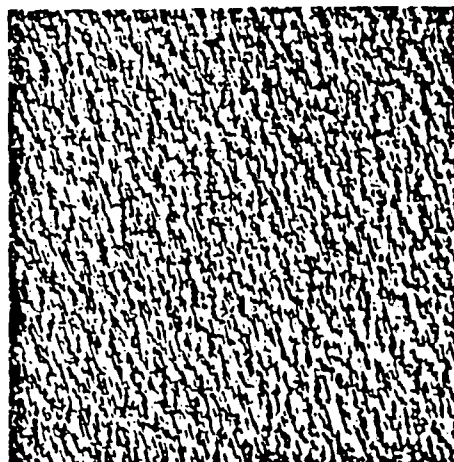
serves two principal purposes. First, it provides a "clean" surface for nucleation of GaAs or AlAs. Second, oxygen-free Si is more ductile than ordinary Si with appreciable oxygen content. It thus can be used as a buffer between the GaAs film and the underlying substrate. Past work on GaAs/AlGaAs lasers has confirmed the importance of the solder used which serves a buffer between the laser and the heat sink and thus relieve the thermal stress in the laser. We have grown GaAs films on Si/sapphire substrates, and detected PL signals. Because sapphire is an insulator, pyrometer does not give an accurate reading of the substrate temperature. We are looking for ways of determining the substrate (top Si surface layer) temperature.

The purpose of studies involving the use of InGaAs in the GaAs/AlGaAs/Si system is many-fold. First, InGaAs forms quantum well with GaAs or AlAs serving as barrier. Such well can be used in lasers to reduce the threshold current. Second, InGaAs is polar while Si is nonpolar. The ionicity values are 0.27 for AlAs, 0.36 for InAs and 0.31 for GaAs. Therefore, now that the degree of ionicity and hence possible charge transfer at the hetero-interface are no longer a major factor, lattice mismatch or misfit stress is the only important factor controlling film growth near the interface. Third, GaAs has a lattice constant ( $5.65 \text{ \AA}$ ) between InAs ( $6.06 \text{ \AA}$ ) and Si ( $5.40 \text{ \AA}$ ). However, InAs has a thermal expansion coefficient ( $5.2 \times 10^{-6}$ ) between GaAs ( $6.4 \times 10^{-6}$ ) and Si ( $2.5 \times 10^{-6}$ ). Therefore, properly placed, InGaAs can be used for stress compensation in GaAs/Si films. Preliminary work on the use of InGaAs for stress compensation has yielded positive results [13] as evidenced from the PL spectrum. The idea is that if a GaAs/Si film is free of stress then InGaAs film grown on top of it should show the same PL peak wavelength as an InGaAs/GaAs film. We are getting close to this stress-free situation. We'll repeat the experiment by varying the

composition and thickness of the InGaAs film to achieve stress-free condition in GaAs/Si film.

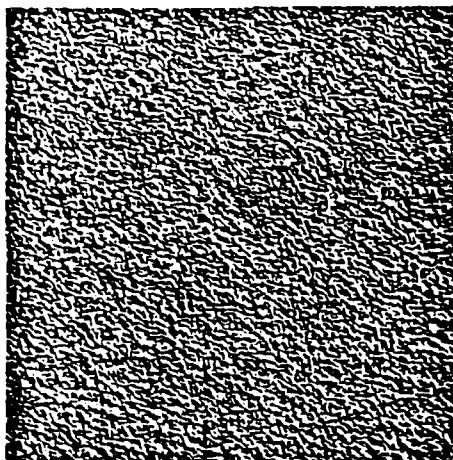
The InGaAs/GaAs SLS or QW has been generally grown on (100) surface. For many applications such as SEED (self electrooptic effect device) it is desirable to have a built-in electric field. This is achieved by growth on (111) plane through piezoelectric effect. So far report on (111) growth has been scanty and the film quality has not been satisfactory. We have studied the growth mechanism of InGaAs on both (111) GaAs and (111) AlAs [11,12]. We find that (111) InGaAs/GaAs growth proceeds quite differently than (100) GaAs/GaAs growth. Specifically, three distinct temperature regimes have been identified, each regime characterized by its own surface reconstruction, growth mechanisms, and film quality. Under conditions of uninterrupted growth on exactly (111) GaAs substrates, only the growth mechanisms of the high temperature regime ( $T_s > 725^\circ\text{C}$ ) have been found to yield material of high optical quality and good surface morphology. However, through the use of appropriately misoriented (or modulated) MBE, the growth mechanisms of the lower temperature regimes may be altered to yield material of high optical quality and good surface morphology [11].

We attribute the change to a proper balance between the rates of Ga-As bond formation, Ga re-evaporation, and Ga-Ga bond formation through Ga migration. Accepting this premise, it is reasonable to expect that Al compounds will improve (111) growth because Al is known to be less mobile and to have a higher enthalpy of reaction with As than Ga. This hypothesis has indeed been borne out by experiments. Figures 2 and 3, taken from the manuscript submitted for publication 12, show the surface morphology of GaAs,  $\text{Al}_{0.67}\text{In}_{0.33}\text{As}$ , and AlAs on (111) GaAs substrates and the



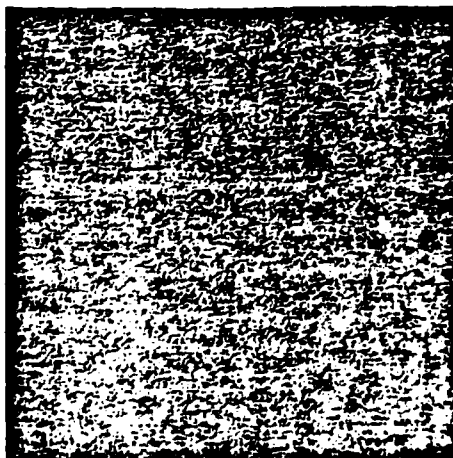
50μm

(a)



50μm

(b)



50μm

(c)

FIG. 2

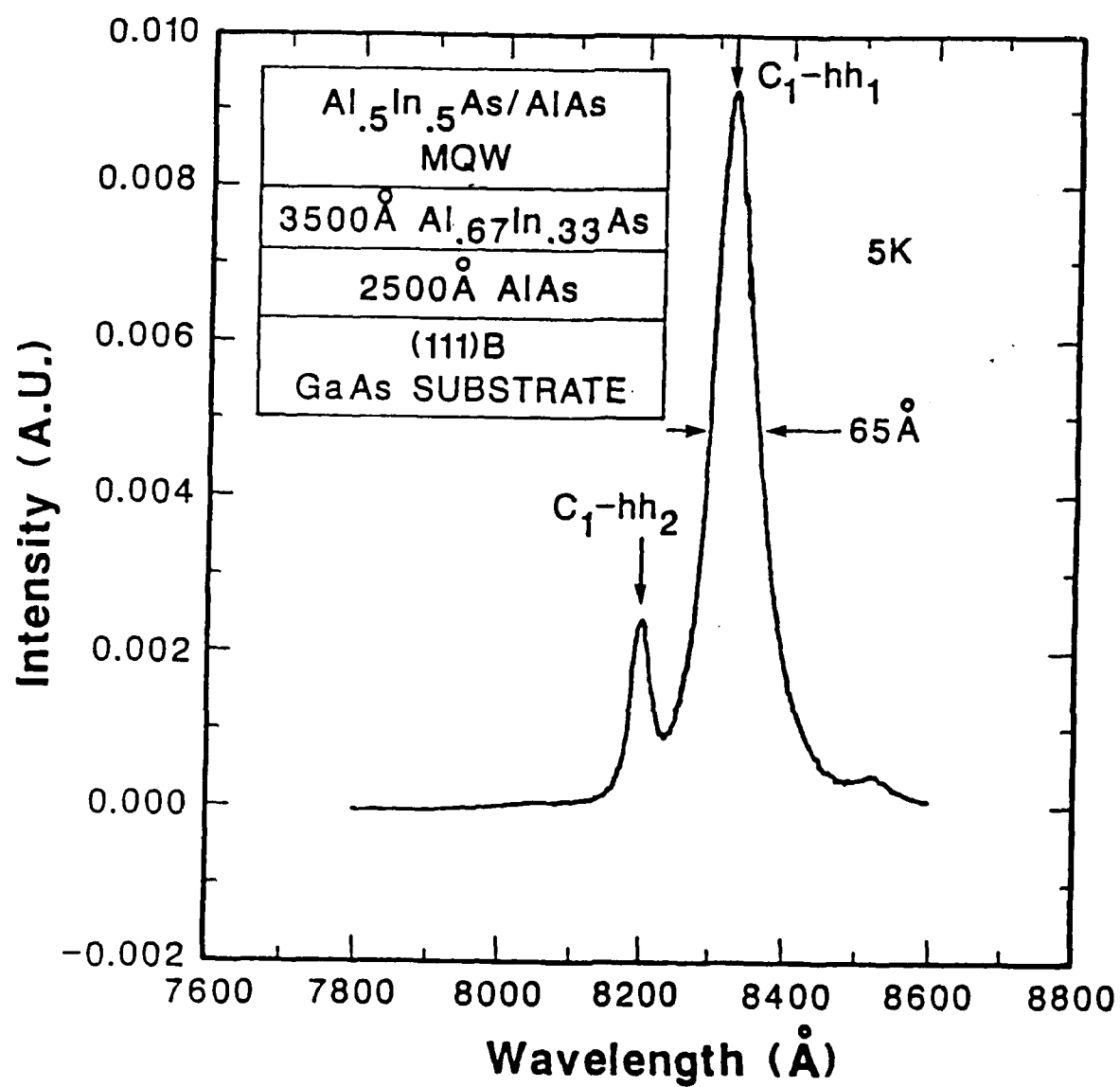


FIG. 3

PL spectrum from  $\text{Al}_{0.5}\text{In}_{0.5}\text{As}/\text{AlAs}$  strained MQW [12] grown on (111) GaAs substrates. We notice that AlAs, AlGaAs, and AlInAs grow much more smoothly than GaAs on (111) GaAs. The growth substrate temperature is only  $600^\circ\text{C}$ . The narrow 5K PL spectral width indicates the high optical quality of the grown film. In field-free QW, the selection rule  $\Delta n=0$  forbids the  $C_1-hh_2$  transition. However, the built-in electric field mixes the parity of the quantum well states and makes the  $C_1-hh_2$  transition observable.

Three Ph.D. students Patrick Harshman, Jay Tu and Hyunchul Sohn (under joint supervision with Eicke Weber) and a "post-doc" Professor Xiaoming Liu of Qinghua University (she returned to Qinghua University in December 1989) participated in various aspects of the work presented above. Dr. H.P. Lee supported by JSEP is now with Belcore in New Jersey. An MS and potential Ph.D. student Ashish Verma joined the group in Fall 1989 and has learned to grow by MBE.

## Publications (April 89-90)

1. H.P. Lee, X. Liu, S. Wang, T. George, and E.R. Weber, "Improvement in the Crystalline Quality of Heteroepitaxial GaAs on Si Films Grown by Modulated Molecular Beam Epitaxy," *Appl. Phys. Lett.*, Vol. 54, p. 2695, June 26, 1989.
2. H.P. Lee, X. Liu, S. Wang, T. George, E.R. Weber, and Z. Liliental-Weber, "Initial Nucleation Studies of Heteroepitaxial GaAs Films on Si Substrates by Modulated MBE," presented at *Material Research Society Spring Meeting* San Diego, April 1989.
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